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Wednesday, August 3, 2022 4:35 PM

Energy order of orbitals

(i) Single electronic species ($H, He^+, Li^{2+}, Be^{3+}$ ......)

E depends only on value of $n \Rightarrow$ shell No.

$n \uparrow$, E of orbital $\uparrow$es.

Energy order

$1s < 2s = 2p < 3s = 3p = 3d < 4s = 4p = 4d = 4f <$ ——

Ground state

Ist Excited state — 4 degenerate orbitals

2nd Excited State $\Rightarrow$ 9 degenerate orbitals

No. of degenerate orbitals in n^{th} shell $= n^2$

(2) for multielectron species (atom or ion)

Energy depends on both n & l value

Bohr-Bury Rule ($n+l$ Rule)

$E \propto (n+l)$ value

If for any two orbitals, $(n+l)$ value is same, then

$\boxed{E \propto n}$

$1s < 2s < 2p < 3s < 3p < 4s < 3d < 4p < 5s$

	1s	2s	2p	3s	3p	4s	3d	4p	5s
$n+l$	$1+0$	$2+0$	$2+1$	$3+0$	$3+1$	$4+0$	$3+2$	$4+1$	$5+0$
	$=1$	$=2$	$=3$	$=3$	$=4$	$=4$	$=5$	$=5$	$=5$

eg: $\boxed{H^\ominus} \Rightarrow 2e$

$H^\ominus = 1s^2\ 2s^0\ 2p^0$

G.S — Ist Ex. State — IInd E.S → 3 degenerate orbitals

#

Method 1

1s
2s 2p
3s 3p 3d
4s 4p 4d 4f
5s 5p 5d 5f 5g
6s 6p 6d - - - -
7s 7p 7d - - - -
8s 8p - - - - - -

Method 2

$1s < 2s < 2p < 3s < 3p < 4s$

$3d < 4p < 5s < 4d < 5p < 6s$

$4f < 5d < 6p < 7s < 5f < 6d < 7p < 8s < \boxed{5g}$

Filling of ēs in orbitals

Rules

(I) Aufbau's Principle

"orbital having lower energy is filled before orbital having higher energy."

or

orbitals are filled in $\uparrow$ing order of their energy.

Note: 4th Quantum No. (Spin) → Not derived from wavefunction

Spin Quantum No (s) $\Rightarrow \left(\frac{1}{2}\right)$

Each e^- revolves about its own axis

clockwise — or Anticlockwise

$s = +\frac{1}{2}$ — $s = -\frac{1}{2}$

OR

$s = -\frac{1}{2}$ — $s = +\frac{1}{2}$

spin of e^- is represented as

$\boxed{\uparrow \text{ or } \downarrow}$

spin Angular Momentum of one e^- $= \sqrt{|s|(|s|+1)}\ \frac{h}{2\pi}$

$= \sqrt{\frac{1}{2}\left(\frac{1}{2}+1\right)}\ \frac{h}{2\pi}$

$= \frac{\sqrt{3}}{2}\hbar$

(II) Hund's Rule of Maximum Multiplicity

Degenerate orbitals are first singly filled with same parallel spin (clockwise or anticlockwise) & then these ēs are paired with opposite spin such that Maximum spin Multiplicity is achieved.

eg: p^3

[↑|↑|↑] ✓

[↑|↑|↑] ✓ — $|S| = \frac{3}{2}$, $M_s = 4$

[↓|↓|↓] ✓ — $|S| = \left|-\frac{3}{2}\right| = \frac{3}{2}$, $M_s = 4$

[↑|↑|↓] ✗

[↑↓|↑|] ✗ — $|S| = \frac{1}{2}$, $M_s = 2$

[↑|↑|↑] ✗

p^4

[↑|↑|↑↓] ✓

[↓|↓↑|↓] ✓

[↑↓|↑|↓] ✗

p^2

[↑| |↑] ✓ $M_s = 3$

[↑|↑|] ✓ $M_s = 3$

[|↓|↓] ✓ $M_s = 3$

Spin Multiplicity (M_s)

$M_s = 2|S| + 1$

$|S| =$ Total spin $= |\Sigma s|$

p^2 [↑|↑|] — $s = +\frac{1}{2}$, $s = +\frac{1}{2}$

$|S| = \left|+\frac{1}{2} + \frac{1}{2}\right| = 1$

$M_s = 2 \times 1 + 1 = 3$

(p^2) [↑↓| |] — $s = +\frac{1}{2}$, $s = -\frac{1}{2}$

$|S| = 0$

$M_s = (2 \times 0) + 1 = 1$